Lagrangian Approaches of Dirac and Feynman to Quantum Mechanics

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February 2, 2008

Abstract

A unified exposition of the Lagrangian approach to quantum mechanics is presented, embodying the main features of the approaches of Dirac and of Feynman. The arguments of the exposition address the relation of the Lagrangian approach to the Hamiltonian operator and how the correspondence principle fits into each context.

1 Introduction

The differential equation of Schrödinger, deduced from the Hamiltonian of a corresponding classical system, formed the central feature of the development of quantum mechanics. Dirac took up what corresponds in the quantum theory to the Lagrangian method of classical mechanics [1]. Dirac took over the ideas rather than the equations, provided by the Lagrangian. Feynman raised this issue in his development of quantum electrodynamics [2]. The physical idea of Dirac was there put into the form of an integral equation. But the approach of Feynman differs so profoundly in formulation from that of Dirac. In Feynman's version the integral equation has been essentially a new formulation of quantum mechanics.

It is very natural to think of the integral eqution as an integral form of the Schrödinger equation. This makes clear the relation of the integral equation to the Schrödinger equation, and brings out the quantum analogue of all the main features of the classical theory of dynamics. However, Feynman's arguments for the integral equation seem to have been guided rather by the desired result than by Dirac's idea. In this paper, I wish to present a unified exposition of the Lagrangian approaches of Dirac and of Feynman to quantum mechanics. The integral equation, introduced by Feynman, is discussed in such a way to complete the original idea of Dirac. For the continuity of discussions arguments in this paper are restricted to one-dimensional cases.

2 Lagrangian approach

In quantum mechanics the action function S has been used for the time integral of the Lagrangian. But the integral is called Hamilton's principal function in classical mechanics. The principle of least action states that the path of a particle is the one of least action out of all the possible paths that do not alter the end points. The path of a particle may be defined by giving only the succession of points x_i through which the particle passes at successive times t_i: $x_i = x(t_i)$. The action can then be written

$$S = \sum_{i=1}^{n-1} S(x_{i+1}, x_i), \tag{1}$$

where

$$S(x_{i+1}, x_i) = \int_{t_i}^{t_{i+1}} L(x(t), \dot{x}(t))\, dt.$$

In classical mechanics the dynamical variables at time t' are connected with their values at time t by a contact transformation. The transformation equations are

$$\frac{\partial}{\partial x} S(x, x') = p \quad \text{and} \quad -\frac{\partial}{\partial x'} S(x, x') = p'. \tag{2}$$

The action S is a function of the coordinates, the constant momenta, and the time. The transformation equations relate the constant momenta with the initial values of coordinates and momenta, thus enabling one to evaluate the constant momenta in terms of the specific initial conditions of the problem. The action function is the generator of a contact transformation to coordinates and constant momenta.

In quantum mechanics the dynamical variables at time t' are connected with their values at time t by a unitary transformation. The transformation equations are

$$\frac{\hbar}{i}\frac{\partial}{\partial x} < x|x' > = p < x|x' > \quad \text{and} \quad -\frac{\hbar}{i}\frac{\partial}{\partial x'} < x|x' > = p' < x|x' > . \tag{3}$$

The expression $< x|x' >$ is just the notation used in the theory of representations. It is for the unitary transformation connecting the two representations when observations are made of the coordinates. If we consider the quantity $< x|x' >$ with x' fixed and x varying, the Schrödinger equation is the condition on the representative, in the moving representation with x diagonal, of the fixed eigenvector corresponding to a state in the Heisenberg picture. As remarked by Dirac, the classical and quantum equations are related in the closed form by putting

$$< x|x' > = e^{iS(x,x')/\hbar}. \tag{4}$$

This is the natural extension of the well-known result that the phase of a wave function corresponds to action function.

Equation (1) is valid only when we substitute for the intermediate x_i their values for the real trajectory, small variations in which values leave S stationary. The corresponding quantum equation is written by (4) as

$$< x_n|x_1 >= \int \cdots \int < x_n|x_{n-1} > dx_{n-1} \cdots < x_3|x_2 > dx_2 < x_2|x_1 >, \quad (5)$$

which follows from the property of basic vectors. It is the process of substituting those values for the intermediate x_i which corresponds to the integrations over all values for the intermediate x_i in (5). The classical requirement that the values of the intermediate x_i shall make S stationary corresponds to the condition in quantum mechanics that all values of the intermediate x_i are important in proportion to their contribution to the integral. The quantum analogue of the action principle is absorbed in the composition law (5).

The composition law (5) may equally be written in the form of a recursive relation

$$< x_{i+1}| = \int < x_{i+1}|x_i > dx_i < x_i| \quad \text{for } i = 2, \cdots, n-1. \quad (6)$$

They describe the developments of a wave function with time. We have here the integral equation in the form

$$\psi(x) = \int < x|x' > \psi(x')\, dx'. \quad (7)$$

Feynman began with a discussion of the integral equation. Equation (7) is easily interpreted physically as the expression of Huygens' principle for matter waves. If the amplitude of ψ is known on a line consisting of all x' at time t', its value at a nearby point x at time t is a sum of contributions from all points of the line at time t'. Each contribution is delayed in phase by an amount proportional to the action it would require to get from all points of the line to the point x along the path of least action.

In Feynman's explanation the kernel $< x|x' >$ is an influence function which gives the effect at any other point x at a time t of a wave function given at x' at an earlier time t'. It describes the manner in which matter waves propagate from its initial position. According to Dirac, the quantity $< x|x' >$ is that solution of the Schrödinger equation for which the coordinates have the values x' at time t'. The square of its modulus is the relative probability of the coordinates having the values x at time t if they have the values x' at time t'. In their explanations, therefore, $< x|x' >$ has been a link relating the two equations, differential and integral. This means that the transformation function is a kind of Green's function for the Schrödinger equation. But there remains the task of showing that the transformation function is indeed a Green's function for the Schrödinger equation. This we do by applying the idea of Dirac to the Hamilton-Jacobi equation.

The Hamilton-Jacobi equation is

$$\frac{\partial S}{\partial t} + H = 0. \quad (8)$$

The action function is the solution of the first-order partial differential equation. From the form of the Hamiltonian, the Hamilton-Jacobi equation can also be written as

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V = 0. \tag{9}$$

By an extension of the argument that led to (3), it is seen that the quantum analogue of (9) has the form

$$\frac{\hbar}{i}\frac{\partial}{\partial t} < x|x' > -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} < x|x' > + V < x|x' >= 0. \tag{10}$$

In putting into (10) the momentum has been treated as a constant. The quantum equation for $< x|$ follows directly from the form of (10), as can be seen when we multiply the equation by $< x'|$ and integrate with respect to x'. It is obvious that the wave function defined by the integral (7) actually satisfies the Schrödinger equation.

In scattering the effect of the scattering center on the free particles is represented by a potential energy which is appreciably different from zero only within a finite region. While the particles may approach from and recede to infinite distance, the potential energy is localized in space and can thus be regarded as an inhomogeneity.

The Hamilton-Jacobi equation for scattering should therefore have the form

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - H_0 = \begin{cases} -V(x) & \text{if } x \to x' \\ 0 & \text{otherwise} \end{cases}, \tag{11}$$

where H_0 is the kinetic energy of the free particle. From this form of the Hamilton-Jacobi equation we may deduce the corresponding quantum equation of the form

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} < x|x' > - H_0 < x|x' >= -V(x')\delta(x - x'). \tag{12}$$

The inhomogeneity of potential energy is the reason for the choice of the δ function instead of the transformation function. With this very reason the quantum equation makes the property of $< x|x' >$ explicit. We see that the form of (12) also fits in completely with Dirac's argument if we assume that

$$< x|x' > \to \delta(x - x') \quad \text{as } x \to x'. \tag{13}$$

Again, we obtain the Schrödinger equation when we multiply (12) with $< x'|$ and integrate over x'. However, it is the inhomogeneous equation in which the potential energy acts as a source of scattered waves. To construct its formal solution, we need a solution of the corresponding homogeneous equation. We denote the solution by $< x|x' >_0$. This is described as satisfying the point source equation

$$\frac{\partial^2}{\partial x^2} < x|x' >_0 - \frac{2m}{\hbar^2} H_0 < x|x' >_0 = -\delta(x - x'). \tag{14}$$

As characteristic for the comparison between (12) and (14), we can write down the relation

$$< x|x' >=< x|x' >_0 \frac{2m}{\hbar^2} V(x'). \tag{15}$$

With $< x|x' >$ given by (15), the integral equation (7) becomes

$$\psi(x) = \psi_0(x) + \frac{2m}{\hbar^2} \int < x|x' >_0 V(x')\psi(x')\, dx', \tag{16}$$

where ψ_0 is the wave function without being scattered. Born showed how the Schrödinger equation for scattering is reformulated as an integral equation. Equation (16) is identical in form with the integral equation introduced by Born. In comparison we identify $< x|x' >_0$ as the Green's function for the Schrödinger equation. In a certain sense we see the transformation function as the Green's function in terms of representations.

For a time dependent perturbation we start with the Hamilton-Jacobi equation of the form

$$\frac{\partial S}{\partial t} + H_0 = \begin{cases} -V(x',t') & \text{if } x,t \to x',t' \\ 0 & \text{otherwise} \end{cases} . \tag{17}$$

This leads to

$$\frac{\hbar}{i}\frac{\partial}{\partial t} < x|x' > + H_0 < x|x' >= -V(x',t')\delta(t-t')\delta(x-x'). \tag{18}$$

To be explicit,

$$\frac{\hbar}{i}\frac{\partial}{\partial t} < x,t|x',t' > + H_0 < x,t|x',t' >= -V(x',t')\delta(t-t')\delta(x-x'). \tag{19}$$

The integral (7) is now extended to include the time integral. In exactly the same manner, we may put the integral (7) in the explicit form

$$\psi(x,t) = \psi_0(x,t) + \frac{i}{\hbar} \int\int < x,t|x',t' >_0 V(x',t')\psi(x',t')\, dt'dx'. \tag{20}$$

This provides an expression for the effect of time dependent perturbations in a form that relativistic invariance is obvious. The invariant form of expression meets what Dirac expected when he took up the question from the Lagrangian formulation of classical mechanics.

In a direct way we may approach the integral equation formulation. Compared to the kinetic energy of a free particle, the potential energy is very local and is momentary. We can thus specify the effect of a perturbing potential by dividing S into two parts,

$$S(x,x') = S_0(x,x') + \int V(x',t')\, dt'. \tag{21}$$

From the definition (4) an expression is readily found for the case in which $V = 0$. The exponential is a physical form of expression for our Green's function, $< x|x' >_0$.

The part of the exponential of (4) which depends upon V can be expanded in a power series. On the other hand, we may expand ψ in terms of V and ψ_0 by iteration of (20). It is of interest to note the equivalence of that power series expansion and this multiple scattering series. The manipulation of the range of integrations accounts for a factor $1/n!$ in the expansion of the exponential, showing the equivalence of the power series and the multiple scattering series [3].

In form the integral (7) is a variational equation. Here the variational problem is to determine the transformation function so that the distribution of the resulting wave function will be a stationary. The variation of the integral (7) gives

$$\delta\psi(x) = \int \delta < x|x' > \psi(x')\, dx'. \tag{22}$$

This is exactly the form of (20), with the variational expression given by

$$\delta < x|x' > = < x|x' >_0 \, \delta S. \tag{23}$$

The variation of S is the difference between S and S_0 and is described by the time integral of a perturbing potential. The equation $\delta\psi = 0$ is then a quantum mechanical statement of the action principle of classical mechanics. If at some initial instant the wave function is given, in words, then at subsequent instants this distribution will change according to the action principle of classical mechanics. When viewed from the present point, the Schrödinger equation is the condition for ψ to take on a stationary distribution.

We identify the Schrödinger equation as the Hamiltonian operator equation. But there is an ambiguity in their correspondence. Because the differential operator acts on everything that stands to the right, the same relation does not always hold between operators as between classical physical quantities. In fact, successive applications of the momentum operator to the wave function give rise to $\nabla \cdot p$ term in addition to the general effect of multiplication of the function by p^2. This is actually so for the harmonic oscillator problem, resulting in zero-point energy. If zero-point energy is a real physical phenomenon, we need a more convincing argument for the Schrödinger equation.

The formal change in the expression for the Hamiltonian required by the transition from classical to quantum physics must be

$$\int \psi^* E\psi \, dx^3 = \int \left\{ \frac{\hbar^2}{2m} (\nabla\psi^*)(\nabla\psi) + \psi^* V \psi \right\} dx^3 \tag{24}$$

from

$$E = \frac{(\nabla S)^2}{2m} + V. \tag{25}$$

It has the form of a variational expression for the expectation values of the energy. The Schrödinger equation appears as the Euler-Lagrange equation derived from a variational principle by the aid of the boundary condition. Formally at least, it is the way in which the Hamiltonian operator equation goes over into the Schrödinger

equation. The question of the formal analogy with the Hamiltonian does not arise in this way. The variational approach must be more than just a matter of academic curiosity.

3 Additional remarks

The approaches of Dirac and Feynman do not appear in standard courses of quantum mechanics [4]. From their own books we learn of the Lagrangian approaches to quantum mechanics [5]. But we are led to a confusion in their separate explanations. Remarks can be made on their discussions from a comparison with the unified approach presented in this paper.

Dirac developed his arguments on the basis of the theory of representations using the δ function. In this theory the quantity $< x|x' >$ is the scalar product in terms of coordinates of the wave function at time t' and the wave function at time t. From the orthogonality theorem we see that this quantity vanishes for $x \neq x'$. Dirac said that we must have

$$< x|x' >= \delta(x - x'). \tag{26}$$

But $< x|$ and $|x' >$ are vectors at different times. The time difference is just the time of propagation of the wave function from x' to x. The argument of the δ function requires that $< x|$ at time t be of the same vector as $|x' >$ at time t'. To be explicit, thus, (26) should read

$$< x|x' >= \delta(x - x') \quad \text{if } t = t'. \tag{27}$$

We then look upon (26) as a limiting property of $< x|x' >$ rather than its property. Dirac's explanation, that $< x|x' >$ with the property (27) is a solution of the Schrödinger equation, can most naturally be understood when we identify $< x|x' >$ as a Green's function in terms of representations for the Schrödinger equation.

Feynman followed Dirac's arguments, but changed his point of view. In his book, finally, Feynman adopted the expression $K(x, t; x', t')$ in place of the notation $< x|x' >$, with the remark "It is clear that the quantity is a kind of Green's function for the Schrödinger equation." The discussion was thus carried out to a point further than that reached by Dirac. While Dirac began with the Schrödinger equation, Feynman derived the Schrödinger equation from the arguments. However, the relation of (7) to the Schrödinger equation was shown by applying it to the simple case of a particle without carrying through a generalized method. The formulation requires an unnatural subdivision of time intervals, and the calculation is only valid to first order in the small time interval. The proof of the equivalence with the Schrödinger equation cannot be completed in his manner.

References

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